REMChlor-MD: A Screening Level Remediation Simulation Model that Considers Matrix Diffusion

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Background/Objectives. Matrix diffusion occurs when groundwater contaminants present in high permeability zones diffuse into adjacent low-permeability zones. The contaminants that have diffused into the low permeability zones can represent a long-term source of contamination following remediation of the high permeability zones due to the phenomena of back diffusion. Current numerical modeling approaches are not able to accurately resolve the local-scale matrix diffusion effects without resorting to extremely fine grids, with gridblocks numbering in the millions.

ESTCP has funded the development of REMChlor-MD, a free screening level model that simulates transport of dissolved chlorinated solvents from a concentrated source zone considering the effects of partial or complete source remediation at some time after the initial release. The model simulates plume transport with matrix diffusion, and can consider enhanced degradation of parent and daughter compounds as a function of space and time in both the high and low permeability zones.

Approach/Activities. REMChlor-MD uses an alternative modeling approach that employs semi-analytical approximations inside each normal (large) numerical gridblock to represent the local-scale matrix diffusion. This method was originally developed in the geothermal reservoir modeling field for simulating transient heat conduction in low permeability cap rocks. With this method, only the high permeability zone is discretized in the numerical model, and the interaction with the low permeability zone is accounted for in a time-dependent source/sink term that is computed analytically in each gridblock at each time-step. The method has been adapted to apply to matrix diffusion in aquifer aquitard systems, as well as in layered, heterogeneous, and fractured media, and the method includes daughter product generation in the low permeability zone.

Results/Lessons Learned. The new method is extremely efficient, and it compares well with exact analytical solutions for matrix diffusion in aquitards, and in rock systems with parallel fractures. The model has been compared favorably with laboratory matrix diffusion experiments in both layered and heterogeneous systems. The model has also been used to reproduce the results of fine-grid conventional numerical simulations of heterogeneous systems at a tiny fraction of the computational effort. The model and interface are currently in Beta testing, and will be publicly released by ESTCP in the summer of 2018.